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CONDENSED MATTER

Energy Spectrum of the Low-Lying States in $Sr_2FeSi_2O_7$ and the Nature of the Magnetoelectric Effect

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A mechanism underlying the magnetoelectric effect is discussed. This mechanism is related to the combined action of an odd crystal field, spin–orbit coupling, and the interaction of the orbital angular momentum with an applied magnetic field. The effective operator describing the spin states of Fe^{2+} ions is obtained. Such operator allows one to interpret the terahertz spectroscopy data and to calculate both the electric field effect on the magnetization and the magnetic field effect on the electric polarization of the sample. It is demonstrated that the magnetoelectric effect is enhanced with a decrease in the energy corresponding to the tetragonal distortion of ligand tetrahedra.

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INTRODUCTION

A search for novel promising materials is one of the most important areas of modern science. Special attention is drawn to materials with the magnetization changing under the effect of an applied electric field, as well as to those with the permittivity affected by the applied magnetic field (potential multiferroics). In the case of transition metal compounds with a nondegenerate ground state, the multiferroics with spiral spin structures related to the antisymmetric exchange interaction of spins are usually discussed [1, 2]. In this paper, we discuss the nature of magnetoelectric coupling in the fundamentally novel class of materials with a *degenerate* ground state of transition metal ions, such as Fe^{2+} and Co^{3+}, in crystals without the inversion symmetry. As a specific example, we consider the $Sr_2FeSi_2O_7$ compound.

Fe^{2+} ions are characterized by a fivefold degenerate ground state and are located within tetrahedra formed by oxygen ions and compressed along the c axis. The symmetry corresponds to the S_4 point group. For $Sr_2FeSi_2O_7$, the Néel temperature is about 5 K [3, 4]. We analyze the following mechanism of transferring the electric field action onto the spins of iron ions.

The odd crystal field formed by oxygen ions mixes the states belonging to the ground $3d^6$ configuration of an iron ion with the states having the opposite parity ($3d^54p$, etc.) and hence induces the coupling of the orbital degrees of freedom with the applied electric field. On the other hand, the orbital angular momentum of iron is related to the spin via the spin–orbit coupling. Thus, the spin corresponding to the $t_2^3e^3(^5E)$ ground state of the iron ion turns out to be related to the electric field.

The described mechanism underlying the coupling between spins and the electric field is rather efficient and, generally speaking, is already being implemented for the description of the electric field effects in the theory of magnetic resonance applied to impurity centers [5]. In the case of a compound with a high concentration of magnetic ions, we have an important additional factor. The couplings of the orbital degrees of freedom to the electric field, on one hand, and to the magnetic field enhanced owing to the exchange interactions of iron ions, on the other hand, lead to a significant increase in the combined magnetoelectric contribution to the free energy resulting from the product of electric and magnetic fields.

EFFECTIVE ENERGY OPERATOR FOR $Fe^{2+}(^5E)$ STATES

The terahertz spectroscopy data on the structure of the energy spectrum of the Fe^{2+} ion are reported in [3]. The results have been interpreted according to the intermediate crystal field scheme using the basis states of the ^5D term. Here, it is more convenient for us to employ the strong crystal field scheme [6]. In this case, the set of basis functions corresponding to the initial approximation becomes smaller. It includes only two orbital states of the ^5D term, namely, $|\vartheta\rangle = |D, M_L = 0\rangle$ and $|\varepsilon\rangle = \{|D, M_L = 2\rangle + |D, M_L = -2\rangle\}/\sqrt{2}$, which